# The Effect of Quadrupolar Interactions within the SAFT Approach

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The use of effective parameters for dipolar and quadrupolar fluids in an equation of state is a common practice. These effective parameters are believed to take into account the electrostatic interactions of molecules, including those with permanent dipoles or higher order polar moments. Nevertheless, it is well known that the explicit inclusion of the dipole-dipole interaction improves the prediction of thermodynamic properties for dipolar fluids. The explicit inclusion of these interactions in molecular based equations of state, such as the Statistical Associating Fluid Theory (SAFT), is a natural improvement over original formulations. The inclusion of dipole-dipole terms in SAFT had recently been carried out by several researchers. Nevertheless, for fluids with "weaker" electrostatic forces, such as quadrupolar forces, effective parameters are still used.

We present a modification of the SAFT equation of state for quadrupolar fluids, which in contrast to previous versions of the SAFT equation, explicitly accounts for the orientational dependence of the intermolecular quadrupolar forces. A single quadrupole-quadrupole term that includes the second and third perturbation terms is used, and higher terms are approximated in the usual way by the Padé approximation. The importance of the explicit inclusion of the quadrupole-quadrupole interaction in the SAFT EOS is shown in this work, through the computation of phase equilibria and volumetric properties at supercritical conditions of quadrupolar fluids ($CO_2$, $N_2$, $C_2H_2$, $C_2H_6$). Both far from and close to the critical region, a significant improvement for PvT lines, volume expansivity, isothermal compressibility and Joule-Thomson inversion curves is obtained, especially in the extended critical region. The results of this work are compared to current standard multiparametric equations of state for these fluids (e.g. Span-Wagner EOS for $CO_2$) that are essentially equivalent to experimental data.